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Vectorial Models of the Young's Modulus of Textured Polycrystalline Material with a Closely Packed Hexagonal Structure

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Abstract. In the Ural Federal University, samples are obtained by the method of 3D-printing based on the agglomeration of Zr or Ti powders under the preclinical study of osseointegration with the use of an innovative implant. This paper presents a comparison of elastic properties of materials with a close-packed hexagonal structure exemplified by vectorial models characterizing the dependence of Young's modulus on direction and crystalline texture.

ELASTIC BEHAVIOR OF A POLYCRYSTALLINE IN THE REUSS APPROXIMATION

For a microinhomogeneous material, stresses and strains are related at each point by Hooke's law written in tensorial form as

$$\sigma_{ij}=C_{ijmn}\varepsilon_{mn} \text{ or } \varepsilon_{ij}=S_{ijmn}\sigma_{mn}. \tag{1}$$

In this equation σ_{ij}, ε_{mn}, C_{ijmn} and S_{ijmn} are stress and strain tensor components, moduli of elasticity and compliance, respectively.

The execution of averaging operation in Eq. (1) gives rise to the following equations:

$$\begin{cases} <\sigma_{ij}> = C^{*}_{ijmn} <\varepsilon_{mn}> = <C_{ijmn}><\varepsilon_{mn}> + <C^{0}_{ijmn}\varepsilon^{0}_{mn}> \\ <\varepsilon_{ij}> = S^{*}_{ijmn} <\sigma_{mn}> = <S_{ijmn}><\sigma_{mn}> + <S^{0}_{ijmn}\sigma^{0}_{mn}>. \end{cases} \tag{2}$$

In the assumption of the uniformity of strains (ε^{0}_{mn}=0) or stresses (σ^{0}_{mn}=0) in the heterogeneous material, using equations (2), we can obtain the values of effective properties ($C^{*}_{ijmn}, S^{*}_{ijmn}$) in the Voigt (V) and Reuss (R) approximations corresponding to the two limitary models of the material

$$(C^{V}_{ijmn}=<C_{ijmn}>, S^{R}_{ijmn}=<S_{ijmn}>).$$

The correlation of the elastic moduli with the compliance coefficients of a single crystal can be written in matrix form as follows:

$$C_{ij}S_{jk}=\delta_{jk}. \tag{3}$$

Unfortunately, this correlation cannot be used for averaged properties of materials with the hexagonal close-packed structure.

In [1], the equations for the compliance coefficients were obtained using the Reuss approximation as follows:

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$$\begin{cases} S_{11}^R = S_{11} - (2S_1 + S_2)\Delta_1 + S_3\Delta_3 \\ S_{22}^R = S_{11} - (2S_1 + S_2)\Delta_2 + S_3\Delta_4 \\ S_{33}^R = S_{11} - (2S_1 + S_2)(1 - \Delta_1 - \Delta_2) + S_3\Delta_5 \\ S_{23}^R = S_{13} + (S_1 - S_3) * \Delta_1 + S_3/2(1 + \Delta_3 - \Delta_4 - \Delta_5) \\ S_{13}^R = S_{13} + (S_1 - S_3) * \Delta_2 + S_3/2(1 + \Delta_4 - \Delta_5 - \Delta_3) \\ S_{12}^R = S_{13} + (S_1 - S_3) * (1 - \Delta_1 - \Delta_2) + S_3/2(1 + \Delta_5 - \Delta_3 - \Delta_4) \\ S_{44}^R = S_{44} + (S_2 - 4S_3) * \Delta_1 + 2S_3(1 + \Delta_3 - \Delta_4 - \Delta_5) \\ S_{55}^R = S_{44} + (S_2 - 4S_3) * \Delta_2 + 2S_3(1 + \Delta_4 - \Delta_5 - \Delta_3) \\ S_{66}^R = S_{44} + (S_2 - 4S_3) * (1 - \Delta_1 - \Delta_2) + 2S_3(1 + \Delta_5 - \Delta_3 - \Delta_4), \end{cases} \tag{4}$$

where S_1=$S_{12} - S_{13}$; S_2=$S_{66} - S_{44}$; S_3=S_{11}+S_{33}− $S_{44} - 2S_{13}$; $S_{11} - S_{12}$=1/2S_{66}; Δ_i denotes textural parameters of polycrystalline with the hexagonal symmetry of the texture. The textural parameters are the quantitative characteristics of a crystalline texture [2]. The textural parameters can be found by the direct integration of the known functions of the orientations distribution obtained from the direct methods of the quantitative textural analysis. The orientation distribution function shows how many times the density of the joint distribution of the Euler angles defining the distribution of the crystallographic axes is different from the function for a randomly oriented material. The model texture can be represented by a set of ideal orientations.

These formulas allow calculating the average values of the moduli of elasticity and the compliance coefficients from the characteristics of single crystals [3] presented in Table 1 and the data on hexagonal axis straggling (table 2).

TABLE 1. Elastic constants, titanium and zirconium at 25 °C, GPa

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
Ti	162	92	69	181	46.7	35
Zr	143.4	72.8	65.3	164.8	32	35.3

TABLE 2. Compliance coefficients in the Reuss approximation, titanium and zirconium at 25 °C, for the prismatic model texture, GPa

	S_{11}^R	S_{22}^R	S_{33}^R	S_{23}^R	S_{13}^R	S_{12}^R	S_{44}^R	S_{55}^R	S_{66}^R
Ti	0.00829	0.00829	0.009626	–0.0033	–0.0033	–0.0019	0.02499	0.024992	0.021413
Zr	0.0091	0.00905	0.010123	–0.0032	–0.0032	–0.0024	0.02979	0.029789	0.03125

Research of the Anisotropy of Young's Modulus

Typically, the anisotropy of the elastic properties of crystals and anisotropic materials is characterized by the dependence of Young's modulus on the direction, although the change is not a complete characterization of the anisotropy of the elastic properties.

Most researches limit themselves to plotting curves of the angular dependence of the Young's modulus in a plane [4].

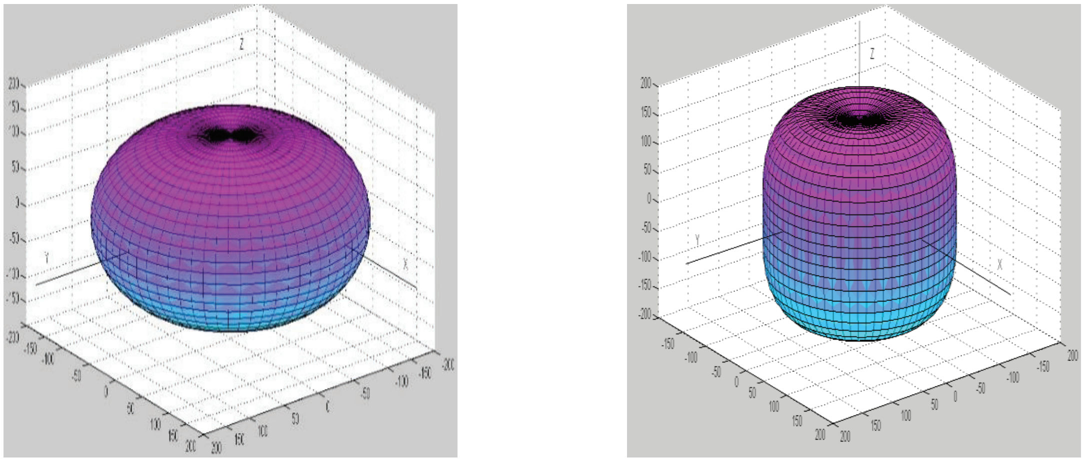
In order to build a 3D vectorial model of the angular dependence of Young's modulus, radius vectors are plotted from a single point; their lengths are proportional to the value characterizing the elastic modulus in this direction. It is known that the basal planes of single crystals with a hexagonal structure in reference to elastic properties are isotropic planes. In this regard, the anisotropy of the elastic properties of such polycrystalline materials is defined only by the orientation of the hexagonal axis. The position of this axis is described by two spherical angles; therefore, their distribution density uniquely determines the anisotropy of the elastic behavior in a polycrystalline material.

The equation of the angular dependence of Young's modulus for metals having a hexagonal lattice is as follows:

$$E^{-1}(\phi,\Upsilon,\varphi,)=S_{11}^R(1-sin^2(\phi)* cos^2(\Upsilon-\varphi))^2+S_{33}^R sin^4(\phi)* cos^4(\Upsilon-\varphi)+(S_{44}^R+2S_{13}^R)*(1-sin^2(\phi)* cos^2(\Upsilon-\varphi))* sin^2(\phi)* cos^2(\Upsilon-\varphi)),$$

where ϕ,Υ and φ are the angles defining the random direction in space.

When the angular dependence of Young's modulus is calculated, it is possible to get the visualization of anisotropy by building the vectorial models.



(a) (b)

FIGURE 1. A vectorial model of Young's modulus for single crystals Ti (a) and Zr (b)

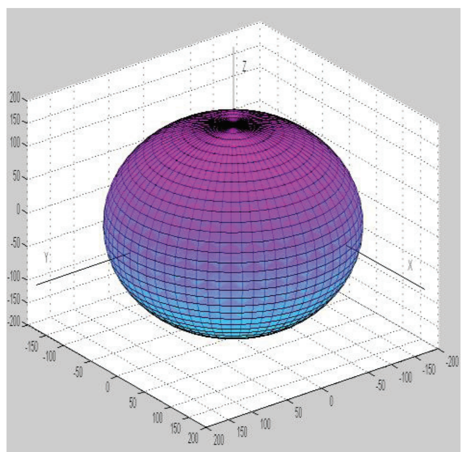


FIGURE 2. A vectorial model of Young's modulus for the quasi-isotropic state of Ti ($\Delta_1 = \Delta_2 = 0.33$; $\Delta_3 = \Delta_4 = \Delta_5 = 0.2$)

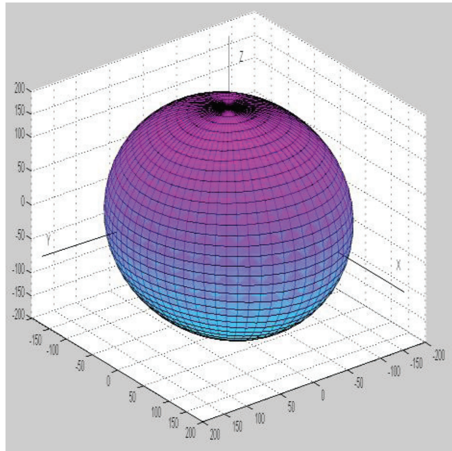


FIGURE 3. A vectorial model of Young's modulus for the model prismatic texture of Delta Ti
($\Delta_1 = \Delta_3 = 1;\ \Delta_3 = \Delta_4 = \Delta_5 = 0$)

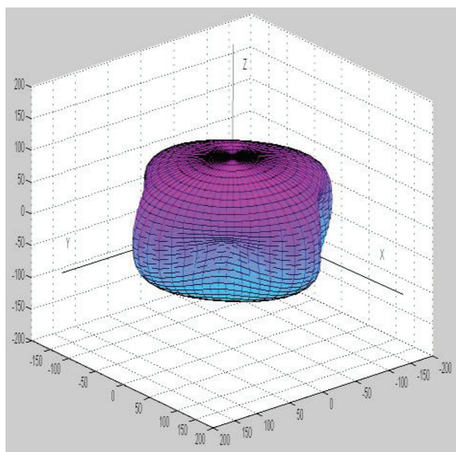


FIGURE 4. A vectorial model of Young's modulus for the texture of titanium sheets
($\Delta_1 = 0.73;\ \Delta_2 = 0.585;\ \Delta_3 = 0.118$
$\Delta_4 = 0.042;\ \Delta_5 = 0.053$) [5]

Figure 1 shows the effect of the elastic behavior of metals on the anisotropy of Young's modulus. According to the technical requirements, titanium-base alloys were selected for the manufacture of implants.

In the case of the quasi-isotropic state of titanium alloys, as it should be, a sphere was obtained as the vectorial model, because the elastic behavior is the same in all directions (see Fig. 2). The same material has different anisotropy of elastic properties at different textural states (Figs 2, 3 and 4). It is possible to separate orientations with extreme values of elastic properties in Figs 3 and 4.

CONCLUSION

From the data on the elastic properties of single crystals having a hexagonal structure and the data on the preferred distribution of crystallographic axes in a polycrystalline material, tensor components of the effective compliance coefficients have been calculated. Ti and Zr alloys, which are the most frequently used for manufacturing implants by 3D printing, have been compared. The advantages of Ti are presented. Vectorial models of different textural states of Ti alloys have been built. In addition, the quasi-isotropic material state, model textures and real textures (the data on which was obtained experimentally by other researchers) have been considered. This paper describes a qualitative difference in the elastic properties, depending on the data about the elastic properties of a single crystal, as well as a significant effect of preferred orientation of crystallographic axes in a polycrystalline on the anisotropy of the Young's modulus of materials that are used in the manufacture of implants. Information on the anisotropy of elastic properties, in particular, Young's modulus, should be considered when selecting the starting materials and methods for sample handling.

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